Disorder effects and electronic conductance in metallic carbon nanotubes

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Abstract

Disorder effects on the density of states and electronic conduction in metallic carbon nanotubes are analyzed by a tight binding model with Gaussian bond disorder. Metallic armchair and zigzag nanotubes are considered. We obtain a conductance which becomes smaller by the factor $1/2 \sim 1/3$ from that of the clean nanotube. This decrease mainly comes from lattice fluctuations of the width which is comparable to thermal fluctuations. We also find that suppression of electronic conductance around the Fermi energy due to disorder is smaller than that of the inner valence (and conduction) band states. This is a consequence of the extended nature of electronic states around the Fermi energy between the valence and conduction bands, and is a property typical of the electronic structures of metallic carbon nanotubes.

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1. Introduction

Recently, carbon nanotubes with cylindrical graphite structures have been intensively investigated. Many interesting experimental as well as theoretical researches have been performed (see reviews [1,2] for example), and the fundamental metallic and semiconducting behaviors of single wall nanotubes predicted by theories [3-8] have been clarified in tunneling spectroscopy experiments [9,10].

Measurements of transport properties of single and multi wall nanotubes depend largely on various factors including sample quality, experimental conditions, and so on. Such factors make experimental interpretations difficult. However, several interesting fundamental properties have been found. Magnetoconductance depending on magnetic field has been measured for multi wall nanotubes, and has been interpreted in terms of two dimensional weak localization and universal conductance fluctuations in mesoscopic conductors [11]. Single electron tunneling experiments of ropes of single wall carbon nanotubes have been performed, and discrete energy levels of nanotubes between metallic contacts contribute to the single electron tunneling processes [12]. Electron correlation effects in the single electron tunneling have also been observed [13]. Furthermore, quantized conductance by the multiples of the unit conductance $2e^2/h = (12.9\mathrm{k}\Omega)^{-1}$ has been measured for multi wall carbon nanotubes [14].

In view of the experimental developments of conduction properties, it is interesting to investigate basic properties of single and multi wall carbon nanotubes theoretically. For conduction properties, interplay between disorder and possibility of long ballistic conduction has been studied [15]. The Landauer formula [16] has been used to calculate quantum ballistic transport properties of nanotubes for example in [17,18]. Quantum tunneling of carbon-nanotube-based quantum dots has been studied in [19].

In this paper, we would like to try to apply the Thouless formula [20,21] differently from the works in literatures [17,18], in order to look at possible decrease of the electronic conductance by a bond disorder potential. The origin of the bond disorder potential is the thermal

fluctuations of phonons mainly. This idea has been used in the discussion of disorder effects on the polaron excitations in doped C_{60} systems [22]. We use a tight binding model with Gaussian bond disorder, and finite systems with quite large metallic carbon nanotubes are diagonalized numerically in real space. The electronic conductance calculated by the Thouless formula is averaged over random samples of disorder. The strength of bond disorder is changed within the width whose magnitude is typical to thermal fluctuation of phonons as estimated in C_{60} and carbon nanotubes [8,22].

We will discuss disorder effects on the density of states and electronic conduction in metallic carbon nanotubes, i.e., armchair and metallic zigzag nanotubes [23]. The conductance at the Fermi energy becomes smaller by the factor $1/2 \sim 1/3$ from that of the clean nanotube. This decrease mainly comes from lattice fluctuations of phonons. The suppression of electronic conductance around the Fermi energy due to disorder is smaller than that of the main part of the valence (and conduction) band states. This is due to the extended nature of electronic states around the Fermi energy

This paper is organized as follows. In Sec. II, the tight binding model and the numerical calculation method are explained. Sections III and IV are devoted to the results of metallic armchair and zigzag nanotubes, respectively. The average conductance at the Fermi energy is discussed in Sec. V. The paper is summarized in Sec. VI.

2. Model

Figure 1 shows the way of making general carbon nanotubes and the notations. The lattice points in the honeycomb lattice are labeled by the vector $(m, n) \equiv m\mathbf{a} + n\mathbf{b}$, where $\mathbf{a}$ and $\mathbf{b}$ are the unit vectors. Any structure of nanotubes can be produced by contacting the origin $(0, 0)$ with one of the (m, n) vectors after rolling up the plane of the honeycomb lattice pattern. This vector is used as a name of each nanotube. The electronic structures of a simple tight binding model with nearest neighbor hopping interactions have been found theoretically. When

the origin of the honeycomb lattice pattern is so combined with one of the open circles as to make a nanotube, the metallic properties will be expected because of the presence of the Fermi surface. This case corresponds to the vectors where $m - n$ is a multiple of three. If the origin is combined with the filled circles, there remains a large gap of the order of 1 eV. This type of nanotubes is a semiconductor.

In Fig. 1, the most characteristic pattern in the two dimensional graphite plane, where the coupling between bond alternations and electrons is present, is superposed. We have refered to this pattern as the Kekulé structure [7,8]. The short and long bonds are indicated by the thick and normal lines, respectively. This pattern is commensurate with the lattice structure for the metallic (m, n) nanotubes, and this bond alternation pattern is realized in the adiabatic approximation. However, the strength of the bond alternations is of the order smaller than the experimentally accessible magnitude [8]. The Kekulé bond alternation pattern will be easily distorted by the fluctuations of the phonons from the classical values. Therefore, we can neglect the bond alternation effects in order to discuss disorder effects on electronic conductance of metallic carbon nanotubes.

Our model Hamiltonian is:

$$H = -t \sum_{\langle i,j\rangle,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.}) + \sum_{\langle i,j\rangle,\sigma} \delta t_{i,j} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.}). \tag{1}$$

The first term is the tight binding model with the nearest neighbor hopping interaction t; the sum is taken over neighboring pairs of lattice sites $\langle i, j\rangle$ and spin σ; $c_{j,\sigma}$ is an annihilation operator of an electron with spin σ at the site i. The second term is the bond disorder model, and the hopping interaction $\delta t_{i,j}$ obeys the Gaussian distribution function

$$P(\delta t) = \frac{1}{\sqrt{4\pi} t_s} \exp[-\frac{1}{2}(\frac{\delta t}{t_s})^2] \tag{2}$$

with the strength t_s.

A finite system with the quite large system size N of metallic carbon nanotubes is diagonalized numerically. In this paper, we take $N = 4000$ for (5,5) and (10,10) nanotubes, and

$N = 3600$ for the (9,0) nanotube. The electronic conductance calculated by the Thouless formula is averaged over 100 samples of disorder. In order to look at dependences on disorder strengths t_s, we have not taken a larger number of samples. However, dependences on t_s are fairly smooth. So, we can discuss typical behaviors of disorder effects, even though numerical error bars remain with a certain magnitude. The quantity t_s is changed within $0 \leq t_s \leq 0.3t$ Note that quantities with the dimension of energy E are measured in units of t ($\sim$ 2 eV) in this paper. The typical magnitude originating from thermal fluctuation of phonons has been estimated as about $t_s \sim 0.15t$ for C_{60} and carbon nanotubes [8,22]. Therefore, the above range of variations seems reasonable.

3. Armchair nanotubes

Two characteristic structures of the armchair nanotubes with (5,5) and (10,10) geometries are investigated. The number of lattice sites in the unit cell is 20 or 40 for each nanotube. Thus, the system with $N = 4000$ has 200 or 100 unit cells. The diameter of the (5,5) nanotube is similar to that of C_{60}, because this nanotube can be made from C_{60} by iterative addition of 10 carbons between two hemisphere of C_{60} [7]. This diameter is the smallest one observed in experiments. The diameter of the (10,10) nanotube is larger than that of the (5,5) nanotube, but most of the observed nanotubes have diameters similar to that of the (10,10) nanotube.

First, we discuss (5,5) armchair nanotubes. Figure 2 shows the density of states (DOS) and electronic conductance of the clean nanotube. Figures 2 (a) and (b) show the entire DOS and the enlarged DOS of the energy region $-1.5t \leq E \leq 1.5t$, respectively. Figure 2 (c) shows the electronic conductance of the energy region as in Fig. 2 (b). We find several peaks of the conductance at the energies $\pm 0.6t$, $\pm 1.0t$, and $\pm 1.3t$ in Fig. 2 (c) at the corresponding peaks of the DOS of Fig. 2(b). This is the usual results by the Thouless formula, though the peaks are somewhat less sharp. The conductance at the energies less than $-0.6t$ and larger than 0.6, i.e. in the inner valence (conduction) band regions, is around 2.0 in the unit of $2e^2/h$. Here, e

is the unit charge, h is the Planck constant, and the factor 2 comes from spin degeneracy. And, the conductance is around the value 1.0 ($2e^2/h$) in the energy region $-0.6t \leq E \leq 0.6t$.

Figure 3 shows one example of the DOS and electronic conductance of the (5,5) nanotube with the disorder strength $t_s = 0.15t$. In Figs. 3 (a) and (b), the strong one-dimensional peaks in the DOS are broaden and suppressed. However, the flat DOS near the Fermi level does not change so much, because the DOS in these energies is nearly the same. Figure 3 (c) shows the conductance in the energy region $-0.6t \leq E \leq 0.6t$. The conductance at the energies less than $-0.6t$ and larger than $0.6t$, i.e. in the inner conduction (valence) band regions, is around 0.1 in the unit of $2e^2/h$. This magnitude is one order smaller than that in the clean system. On the other hand, the conductance is around the value 0.3 ($2e^2/h$) in the energy region $-0.6t \leq E \leq 0.6t$. This value is of the same order of magnitude as that of the clean system. Therefore, we find that the conductance in the inner valence (conduction) band regions is easily suppressed by the disorder. However, the conductance near the Fermi level is not suppressed so much, since conduction and valence bands are mutually connected in the metallic carbon nanotube, and therefore the Fermi level is located just at the center of the whole energy bands. Then, the disorder effects are smallest at the center of the entire energy bands, which means the extended nature of electronic states around the Fermi energy.

Next, we look at the results of the (10,10) nanotube, whose diameter is typical for the observed nanotubes. Figures 4 and 5 are for the clean nanotube and the nanotube with the disorder $t_s = 0.15t$, respectively. As the diameter of the nanotube becomes larger, the number of peaks in the one dimensional DOS increases in Figs. 4 (a) and 5 (a) from that of Figs. 2 (a) and 3 (a). As the DOS of the clean system is flat in the clean system of Fig. 4 (b), the DOS of the system with disorder does not change apparently as shown in Fig. 5 (b). The conductance of the inner valence (conduction) band regions is suppressed by one order of magnitudes when disorder is taken into account as shown by Figs. 4 (c) and 5 (c). However, the magnitude of the conductance around the Fermi energy remains with the similar value. Such a qualitative difference gives rise to larger conductance around the Fermi energy than that of the inner

valence (conduction) band regions in Fig. 5 (c).

4. Zigzag nanotubes

In this section, we discuss typical behaviors of disorder effects in metallic zigzag nanotubes. As an example, the (9,0) geometry is considered in the calculations. We take the carbon number $N = 3600$ here. As the number of carbons in the unit cell is 36, the system is composed of 100 unit cells.

Figs. 6 (a) and (b) shows the entire DOS and the enlarged DOS near the Fermi energy of the clean (9,0) nanotube. Again, several one dimensional peaks are present in both figures. Figure 6 (c) shows the electronic conductance in the units of $2e^2/h$ of the energy region $-1.6t \leq E \leq 1.6t$. We observe several broad peaks of the conductance at the energies $E = \pm 0.5t, \pm 0.6t, \pm 1.0t$, and $\pm 1.3t$, for example. This is again typical results of the calculations by the Thouless formula. The conductance in the inner valence (conduction) band regions is around 1.2 ($2e^2/h$), and that of the energy region around the Fermi energy is about 0.9 ($2e^2/h$). The discrete peaks are due to the discrete energy meshes, and they are of no importance.

Next, we discuss disorder effects on the DOS and electronic conductance by taking results of one sample data of disorder sets. In Figs. 7 (a) and (b), the one dimensional sharp peaks broaden as well by the disorder of the strength $t_s = 0.15t$. However, the magnitude of the DOS around the Fermi energy $E = 0$ does not change its value. Figure 7 (c) shows the electronic conductance of the same disorder sample. The magnitude of the conductance in the inner valence (conduction) band regions is around 0.3 ($2e^2/h$), and this is apparently decreased from that of the clean system. But, the conductance near the Fermi energy is about 0.5 ($2e^2/h$), and is of the same order of the magnitudes with that of the clean system. This is due to the relatively extended nature of the wave functions around the Fermi energy.

Therefore, the qualitative properties of disorder effects on the DOS and the electronic conductivity do not depend on whether the carbon nanotubes are armchair or zigzag type.

5. Disorder strength dependence

In the previous sections, we have looked at the disorder effects by showing the DOS and the conductance data of one disorder sample with $t_s = 0.15t$ for the three geometries of metallic carbon nanotubes. In this section, we concentrate on the conductance at the Fermi energy $E = 0$, and look at the dependence on the disorder strength t_s. Sample average is taken over 100 disorder samples. We have taken relatively larger system sizes, so we cannot take larger sample numbers. However, the average data seem relatively smooth in order to consider disorder strength dependences.

Figure 8 shows the average conductance at $E = 0$ as a function of t_s. The squares, circles, and triangles are for (5,5), (10,10), and (9,0) nanotubes, respectively. The conductances at $t_s = 0$ are about 0.5, 0.6, and 0.9, in units of $2e^2/h$ for (5,5), (10,10), and (9,0) nanotubes. The magnitude at $t_s = 0.15t$ is at about 0.3 ($2e^2/h$) for the three plots. Therefore, the conductance of (5,5) nanotube decreases by the factor about 1/1.6. The conductance of the (10,10) nanotube decreases by the factor about 1/2. The conductance of the (9,0) nanotube decreases by the factor about 1/3. Thus, the electronic conductance of the realistic system with thermal fluctuations of phonons might be decreased by the factor $1/2 \sim 1/3$, naturally.

The extended nature of electronic states at the Fermi energy will contribute to several interesting transport properties observed in experiments. The ballistic conduction [14] and the quantum single electron tunneling [12] are several examples of the recent experiments of carbon nanotubes. We expect further developments of experimental transport studies, which will promote theoretical investigations of carbon nanotubes as well.

6. Summary

Disorder effects on density of states and electronic conduction in metallic carbon nanotubes have been analyzed by a tight binding model with Gaussian bond disorder. Metallic armchair and zigzag nanotubes have been considered. We have obtained a conductance which becomes

smaller by the factor $1/2 \sim 1/3$ from that of the clean nanotube. This decrease mainly comes from lattice fluctuations of the width which is comparable to thermal fluctuations. We have also found that the suppression of electronic conductance around the Fermi energy due to disorder is smaller than that of the inner valence (and conduction) band states. This is due to the extended nature of electronic states around the Fermi energy

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Figure Captions

Fig. 1. Possible way of making helical and nonhelical tubules. The open and closed circles indicate the metallic and semiconducting behaviors of the tight binding model, respectively. The Kekulé structure is superposed on the honeycomb lattice pattern.

Fig. 2. Density of states (DOS) and electronic conductance of the clean (5,5) nanotube. Figures 2 (a) and (b) show the entire DOS and the enlarged DOS of the energy region $-1.5t \leq E \leq 1.5t$, respectively. Figure 2 (c) shows the electronic conductance in units of $2e^2/h$ of the low energy regions.

Fig. 3. Density of states (DOS) and electronic conductance of one sample of the (5,5) nanotube with the disorder strength $t_s = 0.15t$. Figures 3 (a) and (b) show the entire DOS and the enlarged DOS of the energy region $-1.5t \leq E \leq 1.5t$, respectively. Figure 3 (c) shows the electronic conductance in units of $2e^2/h$ of the low energy regions.

Fig. 4. Density of states (DOS) and electronic conductance of the clean (10,10) nanotube. Figures 4 (a) and (b) show the entire DOS and the enlarged DOS of the energy region $-1.5t \leq E \leq 1.5t$, respectively. Figure 4 (c) shows the electronic conductance in units of $2e^2/h$ of the low energy regions.

Fig. 5. Density of states (DOS) and electronic conductance of one sample of the (10,10) nanotube with the disorder strength $t_s = 0.15t$. Figures 5 (a) and (b) show the entire DOS and the enlarged DOS of the energy region $-1.5t \leq E \leq 1.5t$, respectively. Figure 5 (c) shows the electronic conductance in units of $2e^2/h$ of the low energy regions.

Fig. 6. Density of states (DOS) and electronic conductance of the clean (9,0) nanotube. Figures

6 (a) and (b) show the entire DOS and the enlarged DOS of the energy region $-1.5t \leq E \leq 1.5t$, respectively. Figure 6 (c) shows the electronic conductance in units of $2e^2/h$ of the low energy regions.

Fig. 7. Density of states (DOS) and electronic conductance of one sample of the (9,0) nanotube with the disorder strength $t_s = 0.15t$. Figures 7 (a) and (b) show the entire DOS and the enlarged DOS of the energy region $-1.5t \leq E \leq 1.5t$, respectively. Figure 7 (c) shows the electronic conductance in units of $2e^2/h$ of the low energy regions.

Fig. 8. The average conductance at the Fermi energy $E = 0$ as a function of t_s. The squares, circles, and triangles show the numerical data of (5,5), (10,10), and (9,0) nanotubes, respectively.